Computational Materials Discovery: a Dream that is Becoming Reality

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Thanks to powerful evolutionary algorithms, in particular the USPEX method [1-3], it is now possible to predict both the stable compounds and their crystal structures at arbitrary conditions, given just the set of chemical elements. Recent developments include major increase of efficiency and extensions to low-dimensional systems and molecular crystals [4] (which allowed large structures to be handled easily, e.g. Mg(BH4)2 [5] and H2O-H2 [6]) and a new technique called evolutionary metadynamics [7].

Some of the results that I will discuss include:

1. Theoretical and experimental evidence for a new partially ionic phase of boron, γ-B [8] and an insulating and optically transparent form of sodium [9].

2. Predicted stability of "impossible" chemical compounds that become stable under pressure – e.g. Na3Cl, Na2Cl, Na3Cl2, NaCl3, NaCl7 [10], Mg3O2 and MgO2 [11].

3. Novel surface structures (e.g. boron surface reconstructions [12]).

4. Novel dielectric polymers, confirmed by experiment and ready for applications [13].

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